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AFRL-SR-BL-TR-01-

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1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE		3. .	
4. TITLE AND SUBTITLE Numerical Modeling and Analysis of Transient Electromagnetic Wave Propagation and Scattering				5. FUNDING NUMBERS F49620-99-1-0072	
6. AUTHOR(S) Peter G. Petropoulos					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Mathematical Sciences New Jersey Institute of Technology University Heights Newark, NJ 07102				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NM 801 N. Randolph Street Room 732 Arlington, VA 22203-1977				10. SPONSORING/MONITORING AGENCY REPORT NUMBER F49620-99-1-0072	
11. SUPPLEMENTARY NOTES					
12a. DISTRIBUTION AVAILABILITY STATEMENT APPROVED FOR PUBLIC RELEASE, DISTRIBUTION UNLIMITED				12b. DISTRIBUTION STATEMENT (AFOSR) NOTICE OF TRANSMITTAL DTIC. THIS TECHNICAL REPORT HAS BEEN REVIEWED AND IS APPROVED FOR PUBLIC RELEASE LAW AFR 190-12. DISTRIBUTION IS UNLIMITED.	
13. ABSTRACT (Maximum 200 words) In [3] the P1 developed a scaling argument that proved useful in the derivation of reflectionless sponge layers to absorb outgoing time-harmonic waves in numerical solutions of the three-dimensional elliptic Maxwell equations in rectangular, cylindrical, and spherical coordinates. Also, this work developed these reflectionless sponge layers to absorb outgoing transient waves in numerical solutions of the time-domain Maxwell equations and proved that these absorbing layers are described by causal, strongly well-posed hyperbolic systems. A representative result was given for wave scattering by a compact obstacle to demonstrate the many orders of magnitude improvement offered by the developed approach over standard techniques for computational domain truncation.					
14. SUBJECT TERMS				15. NUMBER OF PAGES 12	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT		18. SECURITY CLASSIFICATION OF THIS PAGE		19. SECURITY CLASSIFICATION OF ABSTRACT	
				20. LIMITATION OF ABSTRACT	

20011212 098

Numerical Modeling and Analysis of Transient Electromagnetic Wave Propagation and Scattering

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18 September 2001

Final Report for Period 1 November 1998 - 30 November 2001 (Grant F49620-99-1-0072)

Prepared for
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NM
801 North Randolph St., Room 723
Arlington, VA 22203-1977

1 Technical Summary of Research Accomplished

We will first briefly describe the research results that have already been published in the scientific literature, and then we will provide some details of the remaining publications that resulted from the research effort and are still in press, or to be submitted.

1.1 Summary of Published Research Accomplishments

In [3] the PI developed a scaling argument that proved useful in the derivation of reflectionless sponge layers to absorb outgoing time-harmonic waves in numerical solutions of the three-dimensional elliptic Maxwell equations in rectangular, cylindrical, and spherical coordinates. Also, this work developed these reflectionless sponge layers to absorb outgoing transient waves in numerical solutions of the time-domain Maxwell equations and proved that these absorbing layers are described by causal, strongly well-posed hyperbolic systems. A representative result was given for wave scattering by a compact obstacle to demonstrate the many orders of magnitude improvement offered by the developed approach over standard techniques for computational domain truncation.

In [1], the spherical coordinates case derived in [3] was further explored by the PI and his collaborators. Significantly, that case was compared to the Grote-Keller exact nonreflecting boundary condition which is available for the spherical coordinates case. We found that the reflectionless sponge layer of [3] produces numerical reflection that is of the same order as that produced by the exact condition. Also, we determined via numerical experiments that while the exact condition's performance depends critically in the discretization parameters used in the computational domain, the performance of the reflectionless sponge layer is not thus hampered. Further numerical experiments showed that the reflectionless sponge layer of [3] can produce the same level of spurious reflection as the exact condition in scattering problems but with smaller computational cost. It must be noted here that the numerical implementation of an exact absorbing boundary condition requires that the problem to be solved is spatially periodic in the directions tangential to the surface on which the condition is imposed; the exact conditions are useful only for the case of problems posed in polar coordinates (they cannot be imposed to close a cylindrical computational domain that is not periodic in the \hat{z} direction), in spherical coordinates, and in rectangular coordinates and then only for problems that are periodic in one direction (for two-dimensional problems) or in two directions (for three-dimensional problems). If the reflectionless sponge layer can produce similar spurious reflection as the exact nonreflecting boundary condition in the useful cases where it applies, and do so with a similar computational cost, then the ability of the reflectionless sponge layer to close computations for fully three-dimensional problems in rectangular and cylindrical coordinates makes it superior to exact conditions and renders

it the only absorbing condition worth considering in production codes. We explored the other useful case where an exact condition can be numerically implemented in the discussion of [9] below.

In [5] the PI explored the issue where predictions of performance of exact and approximate Absorbing Boundary Conditions (ABC's) do not take into account the fact that in an actual simulation it is numerical waves that are incident on the computational domain boundary where they are imposed. Via a model problem in rectangular coordinates we framed and examined this issue. Then, we studied the reflection produced by discrete local ABCs in cylindrical coordinates using the first-order Bayliss-Turkel operator as a model. We found the analytical reflection coefficient of this ABC significantly underestimates the actual reflection on the grid. Also, we identified the source of the additional error and showed it decayed slowly with increasing resolution. Implications for other ABC's and reflectionless sponge layer were also discussed.

In [6] we considered a model explicit fourth-order staggered finite difference method for the hyperbolic Maxwell's equations. Appropriate fourth-order accurate extrapolation and one-sided difference operators were derived in order to complete the scheme near metal boundaries and dielectric interfaces with overall fourth-order accuracy. An eigenvalue analysis of the overall scheme provided a necessary, but not sufficient, stability condition and indicated long-time stability. Numerical results verified both the stability analysis, and the scheme's fourth-order convergence rate over complex domains that included dielectric interfaces and perfectly conducting surfaces. For a fixed error level, we found the fourth-order scheme is computationally cheaper in comparison to the Yee scheme by more than an order of magnitude. Some open problems encountered in the application of such high-order schemes are also discussed. Additional research effort is required to extend this very promising fourth-order scheme to arbitrarily shaped domains and dielectric interfaces. We must note here that [6] presented the first fourth-order scheme for Maxwell's equations that maintains its fourth-order accuracy when used to solve problems with boundaries and dielectric interfaces.

In [7] we presented an approximation by exponentials of the time-domain surface impedance of a lossy half-space. Gauss-Chebyshev quadrature of order $N - 1$ was employed to approximate an integral representation of the modified Bessel functions comprising the time-domain impedance kernel. An explicit error estimate was then possible to obtain in terms of the physical parameters, the computation time, and the number of quadrature points N . We showed our approximation is as accurate as other approaches which do not come with such an error estimate. The conditions under which the error estimate derived in [7] also applies to some other approximations were investigated.

Finally, in [8], the PI and his collaborators investigated the stability of a thin two-dimensional liquid film when a uniform electric field is applied in a direction parallel to the

initially flat bounding fluid interfaces. We considered the distinct physical effects of surface tension and electrically induced forces for an inviscid, incompressible nonconducting fluid. The film was assumed to be thin enough and the surface forces large enough that gravity could be ignored to leading order. Our aim was to analyze the nonlinear stability of the flow. We achieved this by deriving a set of nonlinear evolution equations for the local film thickness and local horizontal velocity. The equations are valid for waves which are long compared to the average film thickness and for symmetrical interfacial perturbations. We determined that the electric field effects enter non-locally and the resulting system contains a combination of terms which are reminiscent of the Kortweg de-Vries and the Benjamin-Ono equations. Periodic traveling waves were calculated and their behavior studied as the electric field increases. Classes of multimodal solutions of arbitrarily small period were constructed numerically and shown to be unstable to long wave modulational instabilities. The instabilities were found to lead to film rupture. We presented extensive simulations that showed that the presence of the electric field causes a nonlinear stabilization of the flow in that it delays singularity (rupture) formation. We are presently attempting to delineate the range of applicability of this long-wave theory by comparing with numerical solutions of the full problem. Also, the effect of fluid viscosity and electric conduction is being investigated.

1.2 Summary of Research Results to be Published

In [10] we explored local mesh refinement approaches for the explicit staggered finite difference scheme developed by us in [6] to solve the time-dependent Maxwell equations that describe electromagnetic wave propagation over heterogeneous dielectric media. The underlying scheme is second-order accurate in time and fourth-order accurate in space, and we only considered refinements of the spatial mesh. Numerical examples verified the fourth-order accuracy of the refinement strategy, and again indicated long-time stability. We determined that our approach allows the accurate modeling of waves over domains exhibiting large dielectric contrast.

In [9] we explored in detail the reflectionless sponge layer in two-dimensional polar coordinates. This was done because there exist in the literature results on the performance of very high-order local nonreflecting boundary conditions as well as of exact nonreflecting boundary conditions. With numerical experiments we showed the perfectly matched layer in cylindrical coordinates is as accurate as high-order and exact nonreflecting boundary conditions when used to truncate a computational domain inside which the time-domain Maxwell equations are solved with a staggered second-order accurate finite difference method. For fixed discretization parameters and layer width, we found the numerical reflection produced by the discrete layer is accurately predicted by its analytical reflection coefficient for $\sigma_{max} \in (0, \sigma_{max}^c]$, where σ_{max} is the maximum value of the absorption parameter of the

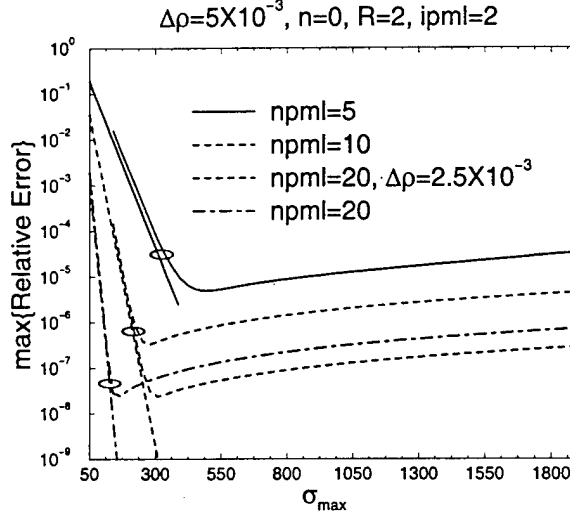


Figure 1: The maximum of the relative error over the time interval $[0, 15]$ as a function of σ_{max} ; The second dashed line corresponds to a $\times 2$ mesh refinement of the $npml = 10$ case. The straight line segments represent the corresponding analytical reflection coefficient, $|R_n^{\Omega_{pml}}|$.

layer. The analytical reflection coefficient of the layer indicates that the spurious reflection converges to zero exponentially fast. Figures 1-5 were obtained for an electric field source designed to excite a cylindrical field mode of a given mode index n . As expected, the reflection produced by the cylindrical reflectionless sponge layer converges to zero exponentially fast with increasing σ_{max} . We also see that, for a fixed spatial mesh size, $\Delta\rho$, the reflection converges to zero exponentially fast with increasing layer width, d_ρ . The most important observation is the fact that the analytical reflection coefficient derived in [3] is a good predictor of the numerical reflection as a function of σ_{max} when that parameter is in a range $(0, \sigma_{max}^c]$. We expect to have obtained similar behavior had we used d_ρ as the variable parameter. Finally, a $\times 2$ mesh refinement (with all other parameters fixed) shows an enlargement of the range of σ_{max} that allows the analytical reflection coefficient to be an accurate predictor of performance. Finally, Fig. 5 indicates the robustness of the discrete layer as a function of the cylindrical mode index n . To produce the Figure we picked the value of σ_{max} that produces the least error for the $npml = 10$ (the number of layers), $ipml = 2$ (the order of loss variation in the layer), $n = 5$ case (see Fig. 2) and then varied the modal index n in the range $[0, 10]$ keeping all other parameters fixed; the error remains $O(10^{-7})$ for $n \leq 5$, and grows for $n > 5$. Clearly, the resolution in the $\hat{\phi}$ direction is not adequate to resolve the harmonics $[6, 10]$. The reduction of the error for $n > 10$ is not a reliable deduction as

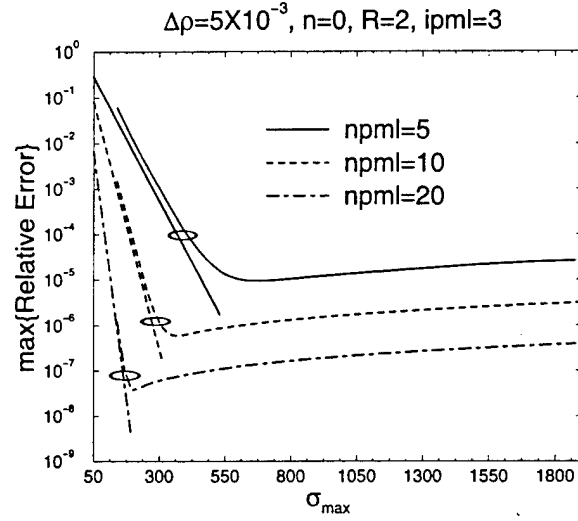


Figure 2: The maximum of the relative error over the time interval $[0, 15]$ as a function of σ_{max} . The straight line segments represent the corresponding analytical reflection coefficient, $|R_n^{\Omega_{pml}}|$.

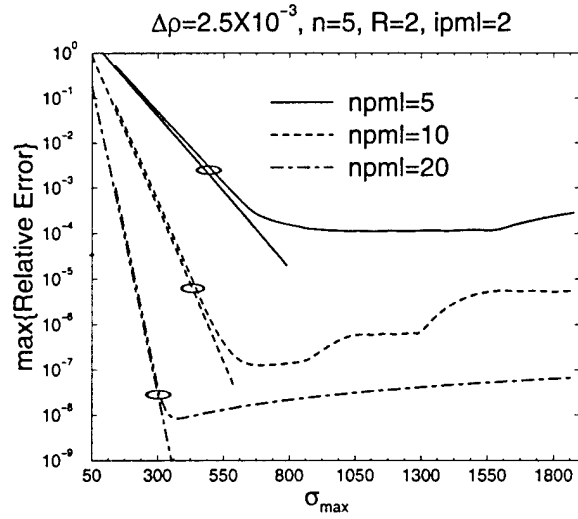


Figure 3: Same as Fig. 2.

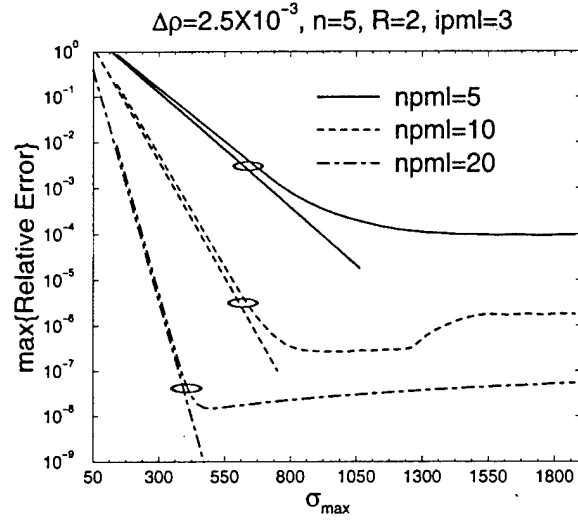


Figure 4: Same as Fig. 2.

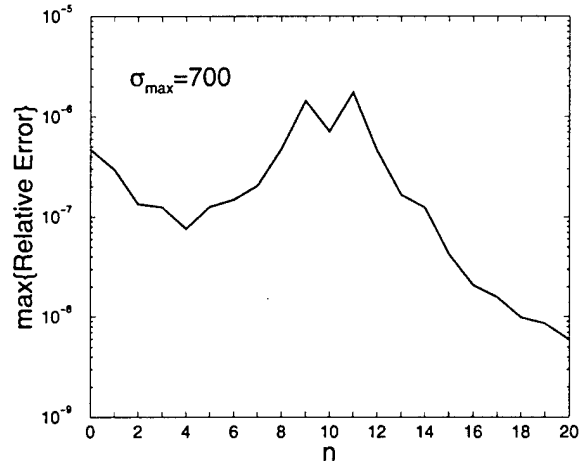


Figure 5: The maximum of the relative error over the time interval $[0, 15]$ for the first 21 cylindrical harmonics.

the error in those cases is obtained with the same $\Delta\rho$ and $\Delta\phi$ (angular resolution). Had we tuned the discrete layer for least error at $n = 10$ we would have seen a similar behavior for the modal index in $[0, 10]$, and then a wavefield composed of 11 cylindrical harmonics would be as effectively absorbed. We have developed an analysis of the discrete layer equations to determine the cutoff value σ_{max}^c given the discretization parameters, and layer width, so that a predetermined amount of reflection of waves exiting the computational domain could be reliably obtained when the layer was used as a nonreflecting boundary condition. This is a topic of ongoing work.

2 Conference Papers and Technical Reports

“A Fourth-Order FD-TD Scheme for Electromagnetics,” Fifth International Conference on Mathematical and Numerical Aspects of Wave Propagation, pp. 883-887, 2000.

“The FD-TD Method: Theory and Applications,” in Applied Computational Electromagnetics: State of the Art and Future Trends, Vol. NATO-ASI Series: SERS. F, pp. 202-242, Springer-Verlag (2000).

“A Non-Dissipative Staggered Fourth-Order Accurate Explicit Finite Difference Scheme for the Time-Domain Maxwell’s Equations, ICASE Technical Report, No. 99-30, NASA/CR-1999-209514, 1999.

3 Presentations

June 1998: Presentation at Workshop in Honor of Prof. V. Ryaben’kii, International Conference on Spectral and High Order Methods, Israel. Title: “Reflectionless Sponge Layers as ABCs for the Numerical Solution of Maxwell’s Equations.”

January 1999: AFOSR Annual Electromagnetics Workshop, San Antonio, TX . Title: “Numerical Dispersion and Absorbing Boundary Conditions.”

April 1999: Division of Scientific Computing, Lucent Technologies, NJ. Title: “Reflectionless Sponge Layers for Computational Electromagnetics.”

June 1999: 5-Day Graduate Seminar, Department of Electrical Engineering, Electrophysics Section, National Technical University of Athens, Greece. Title: “Finite Difference Methods

for Electromagnetics.”

July 1999: ICIAM 99, Edinburgh, Scotland. Title: “The Reflectionless Sponge Layer ABC, A Review.”

January 2000: AFOSR Annual Electromagnetics Workshop, San Antonio, TX. Title: “A Fourth-Order FDTD Scheme for CEM.”

July 2000: 5th SIAM Conference on Mathematical and Numerical Methods in Wave Propagation, Santiago de Compostela, Spain. Title: “A Fourth-Order FDTD Scheme for Electromagnetics.”

September 2000: 1st SIAM Conference on Computational Science & Engineering, Washington DC. Title: “A Fourth-Order Staggered Grid Finite Difference Method for Computational Electromagnetics.”

January 2001: AFOSR Annual Electromagnetics Workshop, San Antonio, TX. Title: “Subgridding a Fourth-Order Staggered Scheme for Maxwell’s Equations.”

July 2001: SIAM Annual Meeting, San Diego, CA. Title: “Fourth-order Accurate FD-TD Schemes for Maxwell’s Equations.”

August 2001: AFOSR FDTD-PIC Workshop, AFRL, Kirtland AFB, NM. Title: “Approximation of Impedance Boundary Conditions Suitable for FDTD Codes and A Fourth-Order Accurate FDTD Method in Domains with Boundaries and Variable Material Properties.”

4 Consultative, Advisory Functions To Other Laboratories And Agencies, and Other Achievements

Throughout the period covered by this report the PI continued his interaction with Dr. T.M. Roberts (Rome Laboratory/ERAA, Hanscom AFB) regarding computational issues that arise in transient electromagnetic wave propagation.

The PI organized a minisymposium titled “Computational Electromagnetics (CEM) in the 21st Century” for the First SIAM Conference on Computational Science and Engineering (CSE00, Washington DC), and a minisymposium titled “Finite-difference time-domain Methods in Electromagnetics” for the 2001 SIAM Annual Meeting (San Diego, CA). Also, he

has acted as a member of the Programme Committee of the Fourth International Workshop on CEM in the Time Domain (Nottingham, UK, 2001).

During the first half of 1999, the PI organized a special graduate student seminar at the National Technical University of Athens, Greece (see above), in which he participated with a one-week long seminar. Also, he edited a special issue on "Absorbing Boundary Conditions for Computational Electromagnetics" for the International Journal of Numerical Modelling: Networks, Circuits and Fields." The issue appeared in vol. 13, no. 5, September-October 2000.

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- [10] A. Yefet and P. G. Petropoulos, "Subgridding a Staggered Fourth-Order FD Scheme for Maxwell's Equations," *J. Computational Physics*, in preparation, 2001.